

OFFICE OF NAVAL RESEARCH

CONTRACT N00014-97-1-0066

R&T Code 33e 1806

Dr. Richard S. Miller

Technical Report No. 98

COMPUTED HEATS OF FORMATION OF THREE DIAZAPENTALENES, AND TWO
GEM-DINITRO/*GEM*-DIFLUORAMINO ANALOGUES OF RDX

by

Peter Politzer, M. Edward Grice and Jane S. Murray

Department of Chemistry
University of New Orleans
New Orleans, LA 70148

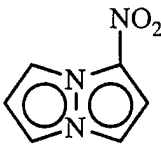
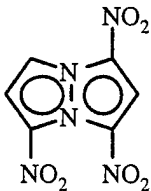
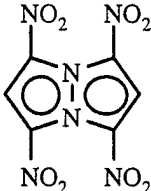
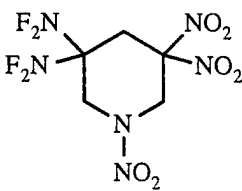
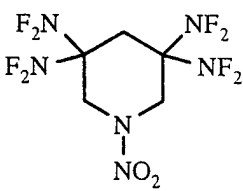
19970131 069

January 24, 1997

Reproduction in whole or in part is permitted for any purpose of the United States Government.

This document has been approved for public release and sale; its distribution is unlimited.

DTIC QUALITY INSPECTED 3

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
<small>Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.</small>				
1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE January 24, 1997		3. REPORT TYPE AND DATES COVERED Technical
4. TITLE AND SUBTITLE Computed Heats of Formation of Three Diazapentalenes and Two Gem-Dinitro/Gem-Difluoramino Analogues of RDX			5. FUNDING NUMBERS N00014-97-1-0066 Dr. Richard S. Miller R&T Code 35e 1806	
6. AUTHOR(S) Peter Politzer, M. Edward Grice and Jane S. Murray				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) University of New Orleans Department of Chemistry New Orleans, Louisiana 70148			8. PERFORMING ORGANIZATION REPORT NUMBER 98	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Office of Naval Research Code 333 800 N. Quincy Street Arlington, VA 22217			10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION/AVAILABILITY STATEMENT Approved for public release. Unlimited distribution.			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words) Computed heats of formation for 1 - 5. <div style="display: flex; justify-content: space-around; align-items: flex-end;"> <div style="text-align: center;">  <p>1</p> </div> <div style="text-align: center;">  <p>2</p> </div> <div style="text-align: center;">  <p>3</p> </div> <div style="text-align: center;">  <p>4</p> </div> <div style="text-align: center;">  <p>5</p> </div> </div> <div style="display: flex; justify-content: space-between; margin-top: 10px;"> <div> <p>1: ΔH_f^{298K} (solid) = 61 kcal/mole = 402 cal/g</p> <p>2: ΔH_f^{298K} (solid) = 67 kcal/mole = 276 cal/g</p> <p>3: ΔH_f^{298K} (solid) = 78 kcal/mole = 273 cal/g</p> </div> <div> <p>4: ΔH_f^{298K} (solid) = -51 kcal/mole = -160 cal/g</p> <p>5: ΔH_f^{298K} (solid) = -77 kcal/mole = -230 cal/g</p> </div> </div>				
14. SUBJECT TERMS heats of formation; diazapentalenes; gem-dinitro/gem-difluoramino analogues of RDX			15. NUMBER OF PAGES	
			16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified	20. LIMITATION OF ABSTRACT Unlimited	

We have used our density functional procedure [1] to compute the heats of formation of the compounds **1** - **5**. **1** and **2** have been prepared by R. Schmitt and J. Bottaro at SRI and **3** is under consideration. The syntheses of **4** and **5** are being pursued by T. Axenrod (CUNY). The vibrational energies were determined from the molecular stoichiometries [2]. The density functional calculations give the gas phase heat of formation, which we convert to the solid state value by subtracting the heat of sublimation. The latter is obtained by means of the relationship that we have developed between the heat of sublimation and the computed electrostatic potential on the molecular surface [3].

Results:

1		$\Delta H_f^{298K}(\text{gas}) = 84 \text{ kcal/mole} = 553 \text{ cal/g}$ $\Delta H_f^{298K}(\text{solid}) = 61 \text{ kcal/mole} = 402 \text{ cal/g}$
2		$\Delta H_f^{298K}(\text{gas}) = 97 \text{ kcal/mole} = 401 \text{ cal/g}$ $\Delta H_f^{298K}(\text{solid}) = 67 \text{ kcal/mole} = 276 \text{ cal/g}$
3		$\Delta H_f^{298K}(\text{gas}) = 113 \text{ kcal/mole} = 394 \text{ cal/g}$ $\Delta H_f^{298K}(\text{solid}) = 78 \text{ kcal/mole} = 273 \text{ cal/g}$
4		$\Delta H_f^{298K}(\text{gas}) = -13 \text{ kcal/mole} = -42 \text{ cal/g}$ $\Delta H_f^{298K}(\text{solid}) = -51 \text{ kcal/mole} = -160 \text{ cal/g}$
5		$\Delta H_f^{298K}(\text{gas}) = -40 \text{ kcal/mole} = -120 \text{ cal/g}$ $\Delta H_f^{298K}(\text{solid}) = -77 \text{ kcal/mole} = -230 \text{ cal/g}$

For comparison, the experimental gas phase ΔH_f^{298K} value for RDX is 206 cal/g [4,5].

References:

1. D. Habibollahzadeh, M. E. Grice, M. C. Concha, J. S. Murray and P. Politzer, *J. Comp. Chem.* **16**, 654 (1995).
2. M. E. Grice and P. Politzer, *Chem. Phys. Lett.* **244**, 295 (1995).
3. P. Politzer, J. S. Murray, M. E. Grice, M. DeSalvo and E. Miller, *Mol. Phys.* in press.
4. D. R. Stull, E. F. Westrum and G. C. Sinke, *The Chemical Thermodynamics of Organic Compounds*, Wiley, New York, 1969.
5. J. M. Rosen and C. Dickinson, *J. Chem. Eng. Data* **14**, 120 (1969).